

# Methodology for simulating the irradiation of the control elements in HFIR

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## INTRODUCTION

The High Flux Isotope Reactor (HFIR) is an 85 MW research reactor operated at Oak Ridge National Laboratory to support neutron scattering experiments, isotope production, and materials irradiation research. HFIR, a pressurized, light-water-cooled and moderated, flux-trap type reactor, is currently fueled with highly enriched uranium. The reactor core consists of a series of concentric annular regions: a central flux trap containing vertical experimental targets surrounded by two fuel elements separated by a thin water region, a region containing two control elements, a beryllium reflector, and a water region to the edge of the pressure vessel, which is located in a pool of water [1].

The two control elements (CEs) in HFIR, the regulating, inner control element (ICE) and the safety, outer control element (OCE), are thin concentric annuli located between the HFIR core and the beryllium reflector. The ICE consists of one annular plate. The OCE is made up of four plates (quadrants) operated in tandem. Each of these plates includes three axial regions with different neutron absorption properties: a “black” strong neutron-absorber region containing  $\text{Eu}_2\text{O}_3$  dispersed in an aluminum matrix, a “gray” moderate neutron-absorber region with tantalum particles in an aluminum matrix, and a “white” region of perforated aluminum [2]. The CEs are present in the core for a large number of reactor cycles, for periods of time that can total up to 1000 days of irradiation. A control element can be removed from the core after a number of irradiation cycles and inserted back in the core after a period of decay time. During irradiation the composition of the poison materials in the CEs changes due to neutron interactions, leading to a change in the properties (cross sections) of these materials. Quantifying these changes throughout the CEs irradiation history will enable a better estimation of the CEs isotopic compositions for use in models of HFIR for various studies and safety assessments.

A methodology has been developed to perform fast simulations of the HFIR CEs’ irradiation history with the purpose of determining their material composition at a given time. This methodology is briefly described in this paper, and results from validation against experimental data available from destructive analysis of an irradiated HFIR control element are presented. The methodology has been applied to determine the CEs’ material compositions at the beginning of cycle (BOC) 400 for use in HFIR safety analysis for this cycle.

## DESCRIPTION OF THE METHODOLOGY

Simulation of the irradiation and decay history of a control rod material is performed using the point depletion and decay code ORIGEN-S in SCALE 6.1 [3]. Though a point depletion code is used, the spatial effects (CEs change locations during an irradiation cycle) are accounted for through the way the one-group microscopic cross sections used in ORIGEN-S calculations are generated.

The cross sections for the CEs’ gray and black regions change during an irradiation cycle compared to the beginning of the cycle, mainly due to the change of the CEs’ axial locations with respect to the core midline. The neutron flux seen by these regions varies, decreasing when the elements are axially moved farther from the core midline toward the core edges. In addition to the change in the neutron flux to which these regions are subjected, there is a resonance self-shielding effect that needs to be accounted for when generating effective one-group cross sections. This effect is due to geometry and material data specific to the CEs (very thin regions of absorbing material surrounded by water and beryllium on one side and fuel or water on the other).

One unique material is considered for each of the gray and black regions in the ICE and OCE for the purpose of generating these cross sections. It is assumed that the effective one-group cross sections for each of the four zones are a function of the CEs’ axial locations. These cross sections are determined, as described further, based on data obtained from a three-dimensional (3-D) Monte Carlo-based depletion simulation [4] of an actual HFIR cycle in which the initial composition of the CEs’ materials is assumed. One set of effective one-group cross sections is generated for each of the black and gray zones to correspond to the CEs’ locations in the core for each day of the irradiation cycle.

### *Model for ORIGEN-S cross-section generation*

New capabilities are available in the SCALE 6.1 release for ORIGEN-S and its associated library management code COUPLE [3]. These new features allow the user to apply multigroup cross sections and neutron flux data from a user-defined reactor physics model (for problem-dependent design and operating conditions) to collapse multigroup cross-section libraries available in SCALE for ORIGEN-S to effective one-group data used in ORIGEN-S calculations. In addition,

user-provided one-group cross sections may be used to override the cross-section data on an existing binary library for ORIGEN-S.

The neutron flux in the gray and black regions of the ICE and OCE was calculated in a multigroup structure as a function of the CEs' axial locations (or cycle time) during the irradiation for an actual HFIR cycle for which detailed operation information is available. The multigroup neutron flux was calculated based on data obtained from the HFIR 3-D depletion simulation with VESTA, a Monte Carlo-based depletion tool that uses MCNP as a transport solver. There are 25 neutron flux data sets for each material zone, one for each of the depletion steps in VESTA, which correspond to 25 different locations of the CEs during the cycle, one value for each cycle day. The neutron flux data were extracted for an energy binning consistent with the 44-group structure used in the SCALE libraries.

The 44-group flux tallied with MCNP is used in the library management code COUPLE to generate the binary library for ORIGEN-S. The COUPLE code builds the problem-dependent one-group effective cross sections by weighting the 44-group SCALE cross-section library with the 44-group user-provided flux. A routine was developed to automatically generate the input files for COUPLE ( $4 \times 25$  files). The binary libraries obtained were checked against cross-section (neutron capture in particular) data available from VESTA simulations. It was observed that for most of the relevant isotopes in the black regions (Eu, Sm, Gd) the variation of the one-group cross sections obtained via COUPLE was in reasonable agreement with the corresponding data available from VESTA. However, a large difference between the COUPLE and VESTA values was seen for the one-group capture cross section of  $^{181}\text{Ta}$  in the gray region. This difference indicates that a 44-group flux (and 44-group cross-section data) as used with the COUPLE input would not be sufficient for this nuclide and cross section and a more refined group flux (and cross-section data) would be needed or that the 44-group cross sections may need a problem-dependent resonance self-shielding treatment. Note that in VESTA, a very fine, 43,000-group flux from the transport calculation is used to obtain one-group cross sections for the depletion calculation.

To resolve the observed difference in the cross sections for  $^{181}\text{Ta}$ , the generation of the cross-section data with COUPLE as described above was slightly modified. The change consisted of using for this isotope the one-group capture cross sections as available from VESTA output files to override the corresponding data on the binary ORIGEN-S library obtained via COUPLE.

The use of these models resulted in generation of 100 binary library files for use with ORIGEN-S: 25 files for each of the gray and black materials in the ICE and OCE, one for each of the 25 axial locations of the CEs with respect to the core midline.

### *ORIGEN-S irradiation simulations for CEs*

Very fast irradiation simulations with ORIGEN-S can be performed for any irradiation history of a CE using the one-group cross section libraries generated as described previously. The total neutron flux in each of the four different CE materials needed as input data for ORIGEN-S is calculated from the MCNP tallies, along with the 44-group flux needed to generate the cross sections for each of the 25 CE locations.

A routine was developed to automatically generate the input files for ORIGEN-S (one for each CE material) for any provided irradiation history data. The irradiation history data include the number of cycles the material was irradiated, the duration of the cycle, and the decay time between two periods of irradiation.

The methodology described above can be also applied to other regions in the reactor for which the effect of the activation during the irradiation cycle is investigated, such as for the beryllium reflector.

## **RESULTS**

### *Validation of methodology against experimental data*

Measurement data for an irradiated ICE, obtained from destructive analysis, have been reported by Knight and Richt [5]. The data correspond to an irradiation of 48,615 MWd fuel burnup. For the gray region of the ICE, it is reported [5] that 0.7 neutrons had been absorbed for every tantalum atom initially present in this region. Isotopic data are reported for five specimens from the black region of the ICE, selected from locations at 0.5, 2, 5, 10, and 20 in with respect to the interface between the gray and black regions. The data include the Eu isotopic composition in at%, as well as the Eu/Gd fraction in wt% for each of the five specimens. No experimental uncertainty is provided for the reported measured data.

Calculations were performed using the methodology described previously to simulate the irradiation of the ICE. An estimation based on the calculated atom densities resulted in a value of 0.71 for the number of neutrons absorbed per tantalum atom initially present in the gray region. This value is in very good agreement with the value based on experimental data and is consistent with the value estimated using a different method [2].

A direct comparison of the calculated and experimental data reported for the black region is not possible, as the measured data are reported as a function of the spatial location inside the black region, whereas the irradiation simulation methodology in this work considers one material only for the black region, and the results for the isotopic compositions are determined as average values over the region (no spatial dependence). However, to facilitate some level of comparison, region-averaged values were estimated from the reported experimental

data by integrating the available curves representing the isotopic compositions as a function of distance [5]. A comparison of these data with the data obtained from simulation is shown in Table I. The agreement is reasonable, considering the approximation made to estimate region-average values based on measured data for the isotopic composition. The comparison of the region-averaged calculated Eu–Gd weight fractions to values inferred based on measured data shows a good agreement between experiment and calculation.

Table I. Calculated-to-measured CE isotopic data

Eu isotopic composition (at %)			
Isotope	Calculated	Measured	Difference
Eu-151	34.18	37.83	-3.65
Eu-153	54.58	54.91	-0.33
Eu-152	7.98	3.75	4.23
Eu-154	3.00	2.60	0.40
Eu-155	0.26	0.91	-0.65
Eu–Gd fractions (wt %)			
Element	Calculated	Measured	Difference
Eu	95.3	94.4	0.9
Gd	4.7	5.6	-0.9

The methodology was applied to estimate the composition of the CEs' materials at BOC 400. A detailed irradiation history was available for the OCE. The OCE was inserted in the core in cycle 390 with fresh composition, irradiated for seven cycles, to cycle 396, removed from the core during cycles 397 to 399, and reinserted for cycle 400. An incomplete irradiation history was available for the ICE. It is known that it was present in the core continuously since it was inserted with fresh composition in the core to cycle 400. History data for the ICE are available from cycle 388; further, the total ICE irradiation time at BOC 388 is also available. The history data prior to cycle 388 were approximated based on the available information. The determined material composition for CEs was used in the VESTA depletion model for HFIR cycle 400. The cross sections for the Monte Carlo-based depletion were based on ENDF/B-VII data.

#### Importance of accounting for CEs irradiation

The effect of the change in the CEs' compositions (and therefore cross sections) on the variation of  $k_{\text{eff}}$  during cycle 400 is significant with respect to both actual values and shape, as illustrated in Fig. 1. Results from two similar models for HFIR cycle 400 are compared. In the old model, the material compositions of the CEs at BOC 400 were assumed to be fresh compositions, whereas in the new model, the material compositions as determined with the methodology described in this paper were used. As shown, the  $k_{\text{eff}}$  variation as a function of

time for the new composition data is smoother than for the assumed composition data, and the accuracy of calculations at each time step is enhanced (agrees well with critical condition in reactor).

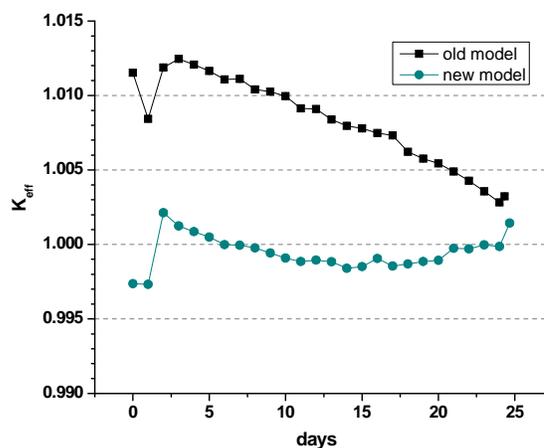


Fig 1. Variation of  $k_{\text{eff}}$  during HFIR cycle 400

## CONCLUSION

A methodology has been developed to perform fast simulations of the HFIR control elements irradiation history with the purpose of determining their material composition at a given time. The approach has been tested against experimental data available from destructive analysis of one HFIR control element and was found to yield good agreement between calculation and measurement. The source of an apparent burnup-dependence of calculated  $k_{\text{eff}}$  has been removed by properly accounting for the control element irradiation history in HFIR depletion simulations.

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